

10/552,015

FILE LAST UPDATED: 23 Mar 2009 (20090323/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

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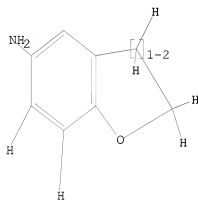
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 18:16:01 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 366191 TO ITERATE

100.0% PROCESSED 366191 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.06

10/923,271

L2 6 SEA SSS FUL L1

L3 41 L2

=> s l3 and py<2003
22983632 PY<2003

L4 17 L3 AND PY<2003

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L4 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:827030 CAPLUS

DOCUMENT NUMBER: 136:177463

TITLE: 6-(4-Benzylpiperazin-1-yl)benzodioxanes as selective ligands at cloned primate dopamine D4 receptors
Hodgetts, Kevin J.; Kieltyka, Andrzej; Brodbeck, Robbin; Tran, Jennifer N.; Wasley, Jan W. F.; Thurkauf, Andrew

CORPORATE SOURCE: Neurogen Corporation, Branford, CT, 06405, USA
SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(12), 3207-3213

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:177463

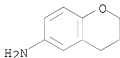
AB A series of novel 6-(4-benzylpiperazin-1-yl)benzodioxanes were prepared and screened at selected dopamine receptor subtypes. 6-(4-[4-Chlorobenzyl]piperazin-1-yl)benzodioxane had high affinity and selectivity for the D4 dopamine receptor subtype and was identified as a D4 antagonist via its attenuation of dopamine-induced GTPγ35S binding at the D4 receptor.

IT 50386-54-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylpiperazinyl benzodioxanes as selective ligands at cloned primate dopamine D4 receptors)

RN 50386-54-4 CAPLUS

CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

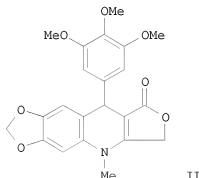
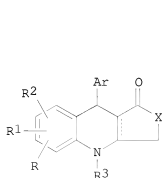
ACCESSION NUMBER: 2001:396489 CAPLUS

DOCUMENT NUMBER: 135:5535

TITLE: Preparation and use of derivatives of dihydrofuro[3,4-b]quinolin-1-ones as anti-tumor agents

INVENTOR(S): Husson, Henri-Philippe; Giorgi-Renault, Sylviane;
 Tratat, Christophe; Atassi, Ghanem; Pierre, Alain;
 Renard, Pierre; Pfeiffer, Bruno
 PATENT ASSIGNEE(S): Adir et Compagnie, Fr.; Les Laboratoires Servier
 SOURCE: Eur. Pat. Appl., 35 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1103554	A1	20010530	EP 2000-403255	20001122 <--
EP 1103554	B1	20030312		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2801310	A1	20010525	FR 1999-14771	19991124 <--
FR 2801310	B1	20040416		
MX 2000011240	A	20020523	MX 2000-11240	20001115 <--
JP 2001151756	A	20010605	JP 2000-355438	20001122 <--
JP 3566649	B2	20040915		
AT 234305	T	20030315	AT 2000-403255	20001122
US 6548515	B1	20030415	US 2000-718917	20001122
ES 2194692	T3	20031201	ES 2000-403255	20001122
NO 2000005922	A	20010525	NO 2000-5922	20001123 <--
HU 2000004704	A2	20011128	HU 2000-4704	20001123 <--
CA 2326710	A1	20010524	CA 2000-2326710	20001124 <--
CA 2326710	C	20060627		
ZA 2000006912	A	20010605	ZA 2000-6912	20001124 <--
CN 1302804	A	20010711	CN 2000-128318	20001124 <--
CN 1157394	C	20040714		
BR 2000005557	A	20010717	BR 2000-5557	20001124 <--
AU 781300	B2	20050512	AU 2000-71825	20001124
HK 1036983	A1	20041231	HK 2001-107838	20011108
PRIORITY APPLN. INFO.: OTHER SOURCE(S): GI		MARPAT 135:5535	FR 1999-14771	A 19991124

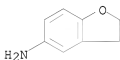


AB Compds. I, their preparation and use as anti-tumor agents are claimed [wherein; R = H, OH or alkoxy; R1, R2 = H, halo, (halo)alkyl, OH, alkoxy, amino, etc.; R3 = H, (hetero)aryl, cycloalkyl, hydroxy, alkoxy, amino, etc.; X = O, S, CH2 or CH2CH2; Ar = (hetero)aryl or arylalkyl]. Over 50 synthetic examples are provided. The process claimed is illustrated by the synthesis of II. N-Methyl-3,4-methylenedioxyaniline was reacted with 3-(3,4,5-trimethoxybenzylidene)-2,4-(3H,5H)-furandione in ethanol at reflux for 30 min to give II. Selected compds. were evaluated for cytotoxicity in L1210, A549 and HT29 cells; IC50 for II was 53, 102 and 104 nM resp. Compds. I were evaluated for in vivo antitumor activity against i.p. implanted murine P388 leukemia cells in BDF1 mice. At doses of 50 mg/kg i.p., II prolonged survival time to 200% of control. A sample formulation is provided.

IT 42933-43-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant; synthesis and use of substituted
 dihydrofuro[3,4-b]quinolin-1-ones as anti-tumor agents)

RN 42933-43-7 CAPLUS

CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2001:58596 CAPLUS

DOCUMENT NUMBER: 134:115968

TITLE: 6-(4-Arylalkylpiperazin-1-yl)benzodioxane and
 6-(4-arylalkylpiperazin-1-yl)chromane derivatives
 useful as subtype-specific dopamine receptor ligands

INVENTOR(S): Tran, Jennifer N.; Thurkauf, Andrew

PATENT ASSIGNEE(S): Neurogen Corporation, USA

SOURCE: U.S., 9 pp.
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

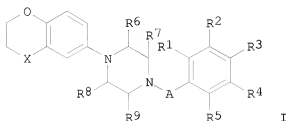
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 6177566	B1	20010123	US 1999-343309	19990630 <--
US 20010005753	A1	20010628	US 2001-761048	20010116 <--
US 6333329	B2	20011225		
US 20020099056	A1	20020725	US 2001-27150	20011220 <--
US 6486164	B2	20021126		

PRIORITY APPLN. INFO.:

US 1998-91250P	P	19980630
US 1999-343309	A1	19990630
US 2001-761048	A1	20010116

OTHER SOURCE(S):
GI

MARPAT 134:115968

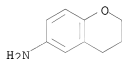


AB The title compds. [I; A = C1-4 alkylene optionally substituted with C1-2 alkyl; R1-R5 = H, halo, C1-6 alkyl, C1-6 alkoxy, C1-4 alkylthio, OH, amino, mono- or dialkylamino, cyano, nitro, CF₃, or CF₃O; R6-R9 = H, C1-6 alkyl; X = O, bond, CH₂, CH₂CH₂, CH₂O] and their pharmaceutically acceptable acid addition salts are disclosed. The compds. are useful for the treatment and/or prevention of neuropsychol. disorders including, but not limited to, schizophrenia, mania, dementia, depression, anxiety, compulsive behavior, substance abuse, Parkinson-like motor disorders, and motion disorders related to the use of neuroleptic agents. As selective ligands for dopamine D₄ receptors, the compds. are expected to be relatively free of neurol. side effects. Approx. 10 salts were prepared and their free bases claimed. Thus, reaction of 1-(1,4-benzodioxan-6-yl)piperazine (preparation given) with 4-fluorobenzyl chloride in the presence of K₂CO₃ in MeCN afforded 34% I [X = O; A = CH₂; R1 = R2 = R4 = R5 = H; R3 = F; R6-R9 = H]. This compound showed a K_i of 11 nM for D₄ receptor binding, vs. K_i values of 3662 nM and >4000 nM for D₃ and D₂ binding, resp.

IT 50386-54-4P, 6-Aminochroman
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of (arylalkylpiperazinyl)benzodioxane and (arylalkylpiperazinyl)chroman derivs. as subtype-specific dopamine receptor ligands)

RN 50386-54-4 CAPLUS

CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:15203 CAPLUS
 DOCUMENT NUMBER: 132:78570
 TITLE: Preparation of
 6-(4-arylalkylpiperazin-1-yl)benzodioxane and

6-(4-arylalkylpiperazin-1-yl)chromane derivatives as
dopamine receptor subtype specific ligands

INVENTOR(S): Tran, Jennifer N.; Thurkauf, Andrew
PATENT ASSIGNEE(S): Neurogen Corporation, USA
SOURCE: PCT Int. Appl., 39 pp.

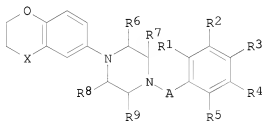
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000000489	A2	20000106	WO 1999-US14426	19990625 <--
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2336089	A1	20000106	CA 1999-2336089	19990625 <--
AU 9947204	A	20000117	AU 1999-47204	19990625 <--
EP 1091949	A2	20010418	EP 1999-930727	19990625 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002519350	T	20020702	JP 2000-557250	19990625 <--
PRIORITY APPLN. INFO.:			US 1998-109242	A 19980630
			WO 1999-US14426	W 19990625

OTHER SOURCE(S): MARPAT 132:78570

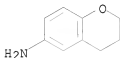
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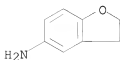
AB The title compds. [I; A = alkylene optionally substituted with alkyl; R1-R5 = H, halo, alkyl, etc.; R6-R9 = H, alkyl; X = O, a bond, alkylene, methyleneoxy] and their pharmaceutically acceptable acid addition salts which are useful for the treatment and/or prevention of neuropsychol. disorders including, but not limited to, schizophrenia, mania, dementia, depression, anxiety, compulsive behavior, substance abuse, Parkinson-like motor disorders and motion disorders related to the use of neuroleptic agents, were prepared. Thus, reacting 1-(1,4-benzodioxan-6-yl)piperazine (preparation given) with 4-fluorobenzyl chloride in the presence of K2CO3 in MeCN afforded 34% I [X = O; A = CH2; R1 = R2 = R4 = R5 = H; R3 = F; R6-R9 = H] which showed Ki of 11 nM against D4 receptor binding vs. Ki of 3662 nM and

>4000 nM against D3 and D2 binding, resp.
 IT 50386-54-4P, 6-Aminochroman
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of 6-(4-arylalkylpiperazin-1-yl)benzodioxane and
 6-(4-arylalkylpiperazin-1-yl)chromane derivs. as dopamine receptor
 subtype specific ligands)
 RN 50386-54-4 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:427209 CAPLUS
 DOCUMENT NUMBER: 125:195464
 ORIGINAL REFERENCE NO.: 125:36607a,36610a
 TITLE: A convenient modification of the Gassman oxindole
 synthesis
 AUTHOR(S): Wright, Stephen W.; McClure, Lester D.; Hageman, David
 L.
 CORPORATE SOURCE: Pfizer Central Research, Groton, CT, 06340, USA
 SOURCE: Tetrahedron Letters (1996), 37(27),
 4631-4634
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A modification of the Gassman oxindole synthesis is described that
 proceeds from anilines XC6H4NH2 (X = H, 4-MeO, 2-Me, 3-MeS, etc.) and Et
 (methylsulfinyl)acetate, using oxalyl chloride to activate the sulfoxide
 to facilitate the formation of the key N - S bonded intermediate. This
 procedure is particularly convenient for reactions carried out on smaller
 scales and for anilines that are susceptible to electrophilic
 halogenation.
 IT 42933-43-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Gassman oxindole synthesis from anilines and Et
 (methylsulfinyl)acetate)
 RN 42933-43-7 CAPLUS
 CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)

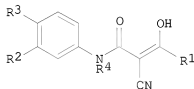


L4 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:777739 CAPLUS
 DOCUMENT NUMBER: 123:198608
 ORIGINAL REFERENCE NO.: 123:35449a,35452a
 TITLE: Preparation of N-aryl-2-cyano-3-hydroxy
 propenamide-derivative antiinflammatory agents
 INVENTOR(S): Evans, Phillip L.; Kuo, Elizabeth Anne
 PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
 SOURCE: Eur. Pat. Appl., 19 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

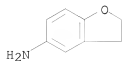
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 652214	A1	19950510	EP 1994-402478	19941103 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07188145	A	19950725	JP 1994-290323	19941101 <--
CA 2135044	A1	19950505	CA 1994-2135044	19941103 <--
PRIORITY APPLN. INFO.: GB 1993-22781			A 19931104	
OTHER SOURCE(S): MARPAT 123:198608				

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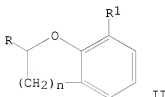
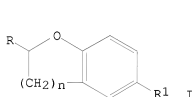


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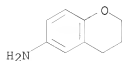
AB The title compds. [I; R1 = alkyl, cycloalkyl, alkenyl, alkynyl; CR2R3 = (un)substituted carbocyclic or heterocyclic ring; R4 = alkyl], useful as antiinflammatory agents, antidiabetic agents (no data), etc. (no data), are prepared and a I-containing formulation presented. Thus, N-[5-(2,3-dihydrobenzofuryl)]-2-cyano-3-cyclopropyl-3-hydroxy-2-propenamide, prepared in 4 steps from 2,3-dihydrobenzofuran, demonstrated 13% inhibition of carrageenan-induced rat-paw edema at 50 mg/kg (p.o.).
 IT 42933-43-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of N-aryl-2-cyano-3-hydroxy propenamide-derivative antiinflammatory agents)
 RN 42933-43-7 CAPLUS
 CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)



L4 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1988:406388 CAPLUS
 DOCUMENT NUMBER: 109:6388
 ORIGINAL REFERENCE NO.: 109:1205a,1208a
 TITLE: Synthesis of amino-substituted 2-methylcoumarans, chromans, benzoxepanes and their N-(alkylamino)acyl derivatives
 AUTHOR(S): Dauksas, V.; Petrauskas, O.; Purvaneckas, G.
 CORPORATE SOURCE: Vil'nyus. Univ., Vilnius, USSR
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1987), (3), 320-4
 CODEN: KGSSAQ; ISSN: 0453-8234
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 109:6388
 GI

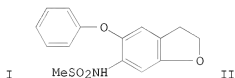
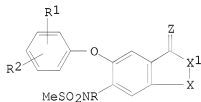


AB Nitration of 2-methylcoumarans, chromans, and benzoxepanes I and II (R = Me, R1 = H, n = 1; R = R1 = H, n = 2,3) gave mixts. of nitro derivs. I and II (R1 = NO2) which were reduced by Fe-Cu in EtOH to give the corresponding amines I and II (R1 = NH2). Acylation of the amines by Me(CH2)3CHBrCOCl gave I and II [R1 = NHCOCHBr(CH2)3Me] which could be aminated by MeNH2 or Et2NH to give I and II [R1 = NHCOCH(NHMe)(CH2)3Me, NHCOCH(NEt2)(CH2)3Me].
 IT 50386-54-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and acylation of)
 RN 50386-54-4 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



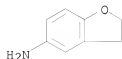
L4 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1983:71912 CAPLUS
 DOCUMENT NUMBER: 98:71912
 ORIGINAL REFERENCE NO.: 98:11003a,11006a
 TITLE: Benzofuran derivatives and their use
 INVENTOR(S): Schroeder, Eberhard; Lehmann, Manfred; Rufer, Clemens;
 Boettcher, Irmgard
 PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.
 SOURCE: Eur. Pat. Appl., 27 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 59884	A1	19820915	EP 1982-101418	19820225 <--
EP 59884	B1	19850522		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DE 3110009	A1	19820930	DE 1981-3110009	19810311 <--
AT 13429	T	19850615	AT 1982-101418	19820225 <--
JP 57203079	A	19821213	JP 1982-37308	19820311 <--
JP 03008350	B	19910205		
US 4411910	A	19831025	US 1982-357344	19820311 <--
PRIORITY APPLN. INFO.:			DE 1981-3110009	A 19810311
			EP 1982-101418	A 19820225
OTHER SOURCE(S):	CASREACT 98:71912; MARPAT 98:71912			
GI				



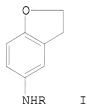
AB Benzofurans I (R = H, Ac; R1, R2 = H, F, Cl; X = O, CH₂; X1 = CH₂, O; Z = O, H₂), useful as inflammation inhibitors, analgesics, antipyretics, diuretics, thrombocyte aggregation inhibitors, anti-ulcer agents, tumor inhibitors, and in treatment of dysmenorrhea and migraine (no data), were prepared. Thus, 2,3-dihydrobenzo[b]furan-5-amine was converted in 7 steps by known methods into methanesulfonamide II.

IT 42933-43-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (N-acetylation of)
 RN 42933-43-7 CAPLUS
 CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)

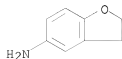


L4 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1983:16571 CAPLUS
 DOCUMENT NUMBER: 98:16571
 ORIGINAL REFERENCE NO.: 98:2683a,2686a
 TITLE: Acetophenetidine analogs
 INVENTOR(S): Blade Font, Arturo; De Mass Rocabayera, Teodoro; Palop
 Palop, Daniel; Escartin Tomas, Pilar
 PATENT ASSIGNEE(S): Laboratorios Frumtost-Prem S. A., Spain
 SOURCE: Span., 16 pp.
 CODEN: SPXXAD
 DOCUMENT TYPE: Patent
 LANGUAGE: Spanish
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 504326	A1	19820601	ES 1981-504326	19810728 <--
PRIORITY APPLN. INFO.: GI			ES 1981-504326	19810728



AB Acylaminobenzofurans I (R = acyl) were prepared Thus
 2,5-HO(AcNH)C₆H₃CH₂NET₂.MeI was treated with 450% excess CH₂N₂ to give 39%
 I (R = Ac) which at 25 mg/kg gave 30.66% inhibition of HOAc-induced
 writhing in mice.
 IT 42933-43-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and acylation of)
 RN 42933-43-7 CAPLUS
 CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)

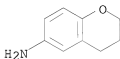


L4 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1982:16951 CAPLUS
 DOCUMENT NUMBER: 96:16951
 ORIGINAL REFERENCE NO.: 96:2827a,2830a
 TITLE: Reagents for detection of urobilinogen in body fluids
 PATENT ASSIGNEE(S): Eiken Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56118670	A	19810917	JP 1980-21692	19800225 <--
JP 63048311	B	19880928		

PRIORITY APPLN. INFO.: JP 1980-21692 A 19800225
 AB Compns. containing phenyldiazonium salts (2,3-dihydroxybenzofuran-5-diazonium tetrafluoroborate, 2,3-dihydroxybenzothiophene-5-diazonium tetrafluoroborate, 1,4-benzodioxane-6-diazonium tetrafluoroborate, 2,3-dihydroxybenzofuran-7-diazonium tetrafluoroborate, 1-acetyl-2,3-dihydroindole-5-diazonium sulfate) and organic acids and(or) inorg. acids are reagents for the detection of urobilinogens in body fluids. As an example, filter papers (Whatman 3MM) were immersed in a solution containing 2,3-dihydroxybenzofuran-5-diazonium tetrafluoroborate, oxalic acid, Na laurylsulfate, MeOH and distilled H2O, and dried at 40°. Development of a pink color is indicative of pos. results. Detection limits were .apprx.0.4 mg/dL.
 IT 50386-54-4
 RL: ANST (Analytical study)
 (diazotization and reaction of, with sodium dodecylbenzenesulfonate)
 RN 50386-54-4 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



L4 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

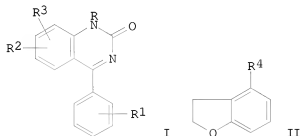
ACCESSION NUMBER: 1977:5484 CAPLUS
 DOCUMENT NUMBER: 86:5484
 ORIGINAL REFERENCE NO.: 86:951a,954a
 TITLE: Tricyclic furoquinazolinones
 INVENTOR(S): Cooke, George A.; Houlihan, William J.
 PATENT ASSIGNEE(S): Sandoz-Wander, Inc., USA
 SOURCE: U.S., 11 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3963717	A	19760615	US 1975-556574	19750310 <--
PRIORITY APPLN. INFO.:			US 1975-556574	19750310

GI



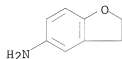
AB Antiinflammatory and analgesic (no data) furoquinazolinones I (R = CHMe2, cyclopropylmethyl, cyclopentylmethyl, CMe3, CH2CMe:CH2, Et; R1 = H, 4-F, 4-CF3, 3-OMe; R2R3 = 7,8-OCH2CH2, 6,7-OCH2CH2, 5,6-CH2CH2O, 6,7-CH2CH2O, 5,6-OCH2CH2, 7,8-CH2CH2O) (38 compds.) were prepared. Thus the benzofuranamine II (R4 = NH2) was treated with Me2CHI, II (R4 = NHCHMe2) treated with NaNCO, II [R4 = N(CHMe2)CONH2] condensed with PhCHO and oxidized with KMnO4 to give I (R = CHMe2, R1 = H, R2R3 = 7,8-OCH2CH2).

IT 42933-43-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isopropyl iodide)

RN 42933-43-7 CAPLUS

CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)



L4 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:526238 CAPLUS

DOCUMENT NUMBER: 79:126238

ORIGINAL REFERENCE NO.: 79:20487a,20490a

TITLE: Nitration of substituted chromans

AUTHOR(S): Brancaccio, G.; Lettieri, G.; Viterbo, R.

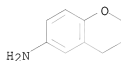
CORPORATE SOURCE: Res. Lab., Richardson-Merrell S.p.A., Naples, Italy

SOURCE: Journal of Heterocyclic Chemistry (1973),

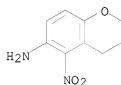
10(4), 623-9

CODEN: JHTCAD; ISSN: 0022-152X

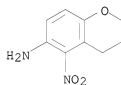
DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The nitration of Cl-, AcNH-, Me-, and NO₂-substituted chromans was studied and the structure of the nitro compds. confirmed by chemical and spectral data.
 IT 50386-54-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Sandmeyer chlorination of)
 RN 50386-54-4 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



IT 50386-66-8P 50603-85-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 50386-66-8 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro-5-nitro- (CA INDEX NAME)



RN 50603-85-5 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro-5-nitro-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L4 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1973:418859 CAPLUS
 DOCUMENT NUMBER: 79:18859
 ORIGINAL REFERENCE NO.: 79:3035a,3038a
 TITLE: Natural and synthetic materials with insect hormone

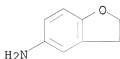
activity. XVI. Synthesis of N-geranylaniline-containing oxygen heterocyclics
 Kahovcova, Jitka; Arnold, Zdenek; Sorm, Frantisek
 AUTHOR(S):
 CORPORATE SOURCE: Cesk. Akad. Ved, Prague, Czech.
 SOURCE: Collection of Czechoslovak Chemical Communications (1973), 38(4), 1165-7
 CODEN: CCCCCK; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The reaction of 4-amino-1,2-methylenedioxybenzene with geranyl bromide in DMF in the presence of anhydrous K₂CO₃ at 70° gave 4-(3,7-dimethyl-2,6-octadienylamino)-1,2-methylenedioxybenzene (I) and 4-[bis(3,7-dimethyl-2,6-octadienyl)amino]-1,2-methylenedioxybenzene. Similar reactions were performed with 5-amino-2,3-dihydrobenzofuran, 5-aminobenzofuran-2-carboxylic acid, 5-amino-benzo-1,3-dioxane, and 5-aminobenzo-1,4-dioxane. From I, 4-(6,7-epoxy-3,7-dimethyl-2-octenylamino)-1,2-methylenedioxybenzene and 4-(3,7-dimethyloctylamino)-1,2-methylenedioxybenzene were also prepared

IT 42933-43-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with geranylbromide)

RN 42933-43-7 CAPLUS

CN 5-Benzofuranamine, 2,3-dihydro- (CA INDEX NAME)



L4 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:4088 CAPLUS

DOCUMENT NUMBER: 64:4088

ORIGINAL REFERENCE NO.: 64:707e-h,708a

TITLE: Amines

PATENT ASSIGNEE(S): F. Hoffmann-La Roche & Co., A.-G.

SOURCE: 9 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6414649	----	19650621	NL 1964-14649	19641216 <--
BE 657234			BE	
FR 1417774			FR	
GB 1043486			GB	
PRIORITY APPLN. INFO.:			CH	19631220

GI For diagram(s), see printed CA Issue.

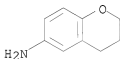
AB Amines with the general formula I, where n is 0-3, R₁, R₂, and R₃ are H or Me, R₄ is an alkyl group, and R₅ is H or an alkyl group, can be prepared from an aminophenol with the general formula II, where R₄' is H or an alkyl group, and R₅' is H, acyl, or an alkyl group, and alcohols of the

general formulas $\text{CH}_2\text{CH}(\text{CH}_3)(\text{OH})[\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)]\text{CH}_3$ or $\text{HOCH}_2\text{CH}:\text{C}(\text{CH}_3)_n\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_n\text{CH}_3$ or their esters. Thus, to a mixture of 11. freshly distilled formic acid (99%) and 120 g. 2,3,5-trimethyl-4-formylaminophenol, 200 g. isophytol was added. With addition of N₂ and refluxing, mixture was stirred for 22 hrs. at 135°. After cooling mixture was poured on 2 kg. ice and a brown oil formed. Yield was 130 g. α -tocopheramine, b_{0.01} 200-3°, absorption maximum at 300 m μ (E11 85), which was acylated and then reduced to give N-ethyl- γ -tocopheramine, a light yellow oil, b_{0.01} 211-14°, uv absorption maximum at 299 m μ (E11 52), n_{24.5D} 1.5086. Similarly obtained, starting with 2,3-dimethyl-4-formylaminophenol, was N-ethyl- γ -tocopheramine, b_{0.05} 195-7°, uv absorption maximum at 238 and 305 m μ (E11 195 and 69), n_{22.5D} 1.5083. In 9 g. dry formic acid, 10 g. α -tocopheramine and 6 g. of a 40% formaldehyde solution were heated for 16 hrs. to boiling. Yield was N,N-dimethyl- γ -tocopheramine, b_{0.02}, 200-5°, n_{23D} 1.5015. Similarly obtained, starting with δ -tocopheramine, was N,N-dimethyl- δ -tocopheramine, b_{0.007} 183-8°, n_{19D} 1.5080, absorption maximum at 244 and 304 m μ (E11 268 and 58). In 1 l. dry formic acid 174 g. N-formyl-2,3-dimethyl-4-aminophenol was dissolved under N₂, 220 g. isophytol was added, and the mixture refluxed for 22 hrs. after which it was poured on 2 kg. ice. Yield was N-formyl- γ -tocopheramine, b_{0.01} 233°, n_{24.5D} 1.5158, which was reduced to yield N-methyl- γ -tocopheramine, a light yellow oil, b. 190-5°, n_{22D} 1.5083, absorption maximum at 306 m μ (E11 74). Similarly obtained, starting with N-formyl- δ -tocopheramine, was N-methyl- δ -tocopheramine, b_{0.005} 189-90°, n_{22.5D} 1.5106, uv absorption maximum at 242 and 309 m μ (E11 225 and 66). Also obtained starting with N-formyl- β -tocopheramine, was N-methyl- β -tocopheramine, b_{0.03} 207-10°, n_{21D} 1.5088, absorption maximum at 234 and 300 m μ (E11 182 and 77). The compds. are useful as anti-oxidants.

IT 50386-54-4, 6-Chromanamine
(derivs.)

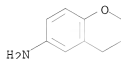
RN 50386-54-4 CAPLUS

CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



L4 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1961:18014 CAPLUS
 DOCUMENT NUMBER: 55:18014
 ORIGINAL REFERENCE NO.: 55:3618h-i,3619a
 TITLE: Aminochroman derivatives
 INVENTOR(S): Hach, V.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	CS 91157		19590715	CS	<--
AB	Chroman (20 g.) treated with 100 ml. 60% HNO ₃ at 15-25° and the mixture (after 10 min. at room temperature) diluted with 100 g. ice and 400 ml. H ₂ O				
	gave 9.5 g. 6-nitrochroman (I), m. 102-3° (EtOH). I (9 g.) was hydrogenated in 100 ml. 96% EtOH over 1 g. Raney Ni at room temperature and normal pressure. Filtration and evaporation gave a quant. yield of 6-aminochroman (II), m. 74° (petr. ether). II (12 g.) in 50 ml. AcOH was cooled to 10° and treated with 12 g. ClCH ₂ COCl. The mixture, diluted with 50 g. AcONa in 150 ml. H ₂ O and filtered, gave 15 g. 6-chloroacetamidochroman (III), m. 125°. Reaction of III with Et ₂ NH gave 90-95% 6-diethylaminoacetamidochroman (IV); HCl salt m. 163°; ethobromide m. 188°. Similarly, III and piperidine gave 6-piperidinoacetamidochroman (V); HCl salt m. 225°. Salts of IV and V were local anesthetic and hypotensive agents.				
IT	50386-54-4P, 6-Chromanamine RL: PREP (Preparation) (preparation of)				
RN	50386-54-4 CAPLUS				
CN	2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)				



L4 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1960:11424 CAPLUS

DOCUMENT NUMBER: 54:11424

ORIGINAL REFERENCE NO.: 54:2322f-i,2323a-b

TITLE: Local anesthetics. XI. Simple chroman derivatives

AUTHOR(S): Hach, V.

CORPORATE SOURCE: Leciva, Dolni Mecholupy, Prague

SOURCE: Collection of Czechoslovak Chemical Communications (1959), 24, 3136-40

CODEN: CCCCAC; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: German

AB cf. C.A. 52, 4652e. 6-(Diethylaminoacetylaminochroman (I), 6-(piperidinoacetylaminochroman (II), and 6-(β-piperidinopropionyl)chroman (III) were prepared as cyclic analogs of p-alkoxy-substituted dialkylaminoacylanilides (IV) and of fallocain (V), resp., and tested in the form of the HCl salts as surface and infiltration anesthetics; their activity, however, was lower than that of IV and V. Introducing 3 hrs. at 0° HBr (prepared from 300 g. Br in H) into 20 g. o-CH₂:CHCH₂C₆H₄OAc, 100 ml. CC1₄ (dried over P₂O₅), and 2 g. Bz₂O₂, keeping the mixture overnight, evaporating the solvent, adding 150 ml. 10% NaOH, extracting the mixture with Et₂O, evaporating the exts., adding 10 g. NaOH, 50 ml. H₂O, and 100 ml. EtOH to the oily residue, boiling the mixture 2.5 hrs.,

diluting with H₂O, extracting with Et₂O, evaporating, and distilling gave chroman (VI),
 b24-27 100-105°, n_D20 1.5480. Adding dropwise and with vigorous agitation in 12 min. at 15-25° 20 g. VI to 100 ml. 60% HNO₃ gave a blue-green mixture which was kept 10 min. at 20° and then poured into 100 g. ice and 400 ml. H₂O; an oily precipitate separated which on addition of 10-15 ml.

EtOH gave 9.5 g. yellow powder of 6-nitrochroman (VII), m. 104° (EtOH). Hydrogenating 1 hr. 9 g. VII, 100 ml. 96% EtOH, and 1 g. Raney Ni at 20° and atmospheric pressure, filtering off the catalyst, and evaporating gave 6-aminochroman (VIII), m. 74° (petr. ether); picrate m. 203° (EtOH); N-Ac derivative (IX) m. 118° (EtOH). Adding in one portion at 10° 12 g. ClCH₂COCl to 12 g. VIII in 50 ml. AcOH and pouring the mixture after 1 min. into 50 g. NaOAc in 150 ml. H₂O gave 15 g. 6-(chloroacetyl amino)chroman (X), m. 125° (EtOH). Treating as usual (C.A. 49, 979e) Et₂NH in C₆H₆ with X gave 90-95% I, b0.3 180-5°, m. 63° (petr. ether); HCl salt (prepared in Et₂O solution) m. 163° (EtOH); picrate m. 201° (EtOH); ethobromide (prepared in acetone solution) m. 188° (EtOH-Et₂O). Similarly was prepared II, b0.5 190-5°; HCl salt m. 225° (EtOH); picrate m. 217° (EtOH). 6-Acetylchroman (XI) was prepared according to Chatelus (C.A. 44, 1975c), m. 43° (petr. ether); oxime (XII) m. 88° (EtOH); thiosemicarbazone m. 219° (EtOH). Heating exactly 7.5 min. at 100-10° 2.5 g. XII, 20 ml. 85% H₃PO₄, and 35 g. P₂O₅, pouring the mixture onto ice, extracting with Et₂O, and evaporating the exts. gave 1.6 g. IX.

Heating 8 hrs. on a steam-bath 8.8 g. XI, 11.1 g. piperidine HCl salt, 8 g. (HCHO)x, and 150 ml. absolute EtOH, keeping the mixture 48 hrs. at 5°, filtering off the precipitate, and washing with 25 ml. EtOH gave 10.3 g. III

HCl

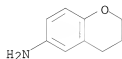
salt, m. 202° (EtOH).

IT 50386-54-4P, 6-Chromanamine 101093-09-8P,
 6-Chromanamine, picrate

RL: PREP (Preparation)
 (preparation of)

RN 50386-54-4 CAPLUS

CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



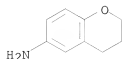
RN 101093-09-8 CAPLUS

CN 2H-1-Benzopyran-6-amine, 3,4-dihydro-, compd. with 2,4,6-trinitrophenol
 (1:1) (CA INDEX NAME)

CM 1

CRN 50386-54-4

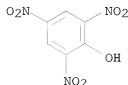
CMF C9 H11 N O



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L4 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1923:8151 CAPLUS

DOCUMENT NUMBER: 17:8151

ORIGINAL REFERENCE NO.: 17:1447f-i,1448a-c

TITLE: Rings through the m- and p-positions of benzene. A study of certain ethers of resorcinol and m-aminophenol

AUTHOR(S): Wilson, W. C.; Adams, Roger

SOURCE: Journal of the American Chemical Society (1923

), 45, 528-40

CODEN: JACSAT; ISSN: 0002-7863

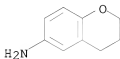
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Attempts to close m- and p-rings, starting from various types of phenol ethers, were unsuccessful. Resorcinol bis- β -bromoethyl ether, from 6H4(ONa)2 and (CH2Br)2 in alc., m. 94.5-5.0°, b9 166-7°. Bis- γ -bromopropyl ether, from 6H4(OH)2, CH2(CH2Br)2 and K2CO3 in Me2CO-H2O, m. 67°, b6 204-6°; with 6H4(ONa)2 there are formed, in addition, 3 other products: the γ -bromopropyl allyl ether, 6H4(OCH2CH:CH2)OCH2CH2CH2Br, m. 88-9°, γ -propyloxyphenyl(allyloxyphenyl)trimethyleneglycol, m. 119-20°, and resorcinol diallyl ether, b12 156-8°, d2020 1.1645, nD20 1.5672. Bis- γ -iodopropyl ether, from the Br compound in aqueous Me2CO with NaI, m. 88-9°, is partly converted by Na in Et2O into the dipropyl ether, also obtained from 6H4(OH)2, PrBr and K2CO3 in Me2CO, b12 127-8°, d2121 1.035, nD33 1.5138. Bis- γ -amylaminopropyl ether, from 6H4(OCH2CH2CH2I)2 and AmNH2 heated alone or in PbMe, b10 249-52°; dihydrochloride, m. 287°. Bis- γ -cyanopropyl ether, from the I compound and NaCN in aqueous alc., b7 236-7°, m. 31-2°, converted by Na in alc. into the bis- δ -aminobutyl ether, b7 208-9° d2020 1.0589, nD26 1.5315, whose dihydrochloride m. 248-9° and monohydrochloride m. 233-4°; the latter, distilled under 7 mm., decomps. into pyrrolidine, m-6H4(OH)2 and resorcinol mono- δ -aminobutyl ether, b8

198-204°, m. 119-9.5° (hydrochloride, m. 159-61°), which in NaOH with p-O₂NC₆H₄COCl gives resorcinol mono-6-p-nitrobenzoylaminobutyl ether p-nitrobenzoate, m. 123-4°, m-Nitrophenyl γ-bromopropyl ether, from O₂NC₆H₄OH, CH₂(CH₂Br)₂ and Na in alc., b₇ 186-8°, d₂₀ 1.513, n_D 1.5700, reduced by SnCl₂-HCl to the m-amino compound, unstable yellow oil (hydrochloride, m. 114-5°), which, refluxed in C₆H₄, gives 6-aminochroman, b₇ 140-2°, d₂₀ 1.1549, n_D 1.5944; hydrochloride, begins to decompose 134°, m. 158-60°; picrate darkens 156-60°, m. 182-3°; chloroplatinate, m. 224-5°, decomp. 227°; benzenesulfonyl derivative, m. 148-8.5°. The diazotized chroman couples with β-naphthol to a red substance, C₁₉H₁₆O₂N₂. m-Nitrophenyl allyl ether, from O₂NC₆H₄OH, CH₂:CHCH₂Br and Na in alc., b₈ 136-7°, m. 31.5-2.0°; m-amino compound, b₅ 120-2°, d₂₀ 1.0891, n_D 1.5708; hydrochloride, m. 145-6°; benzenesulfonyl derivative, m. 83-3.5°. p-Nitrophenol β-bromoethyl ether, from O₂NC₆H₄ONa and (CH₂Br)₂ in H₂O, m. 64°; p-amino compound m. 84°; hydrochloride, m. 196°.

IT 50386-54-4P
 RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
 (Rings through the m- and p-positions of benzene. A study of certain
 ethers of resorcinol and m-aminophenol)
 RN 50386-54-4 CAPLUS
 CN 2H-1-Benzopyran-6-amine, 3,4-dihydro- (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 18:15:27 ON 24 MAR 2009)

FILE 'CAPLUS' ENTERED AT 18:15:37 ON 24 MAR 2009

L1 STRUCTURE UPLOADED
 S L1

FILE 'REGISTRY' ENTERED AT 18:16:00 ON 24 MAR 2009

L2 6 S L1 FULL

FILE 'CAPLUS' ENTERED AT 18:16:07 ON 24 MAR 2009

L3 41 S L2 FULL
 L4 17 S L3 AND PY<2003

=> s 14 and antioxidant

142320 ANTIOXIDANT

L5 0 L4 AND ANTIOXIDANT